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**V ZASEDACÍ MÍSTNOSTI ÚACH
(F III, 1. PATRO) V ŘEŽI**

Libor Kobera

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**EXPERIMENTAL INSIGHT INTO ORGANOMETALLIC
AND INORGANIC MATERIALS: COMPREHENSIVE
XRPD, ssNMR AND DFT STUDY**

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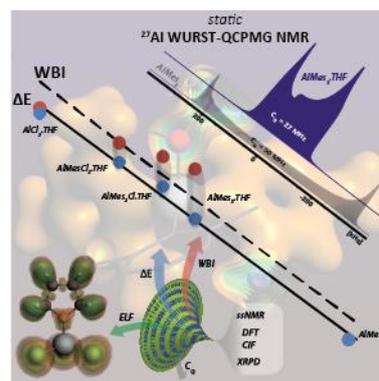
Experimental insight into organometallic and inorganic materials: Comprehensive XRPD, ssNMR and DFT study

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Organometallic and inorganic systems are widely used in chemical industry for ion exchange, sorption, catalysis, molecular sieving, solar cell etc. Experimental/computational strategy based on a solid-state NMR crystallographic approach allows for detailed structural characterization of a wide range of compounds. The NMR crystallography approach (combining of XRPD, ssNMR and DFT calculations) helps to firmly define the exact structure of the investigated system.

Basic characterization is usually accomplished using a combination of the XRPD, ssNMR and DFT study of prepared framework materials. In this presentation not only basic 1D NMR experiments but also advanced ssNMR techniques such as 2D correlation, MQ/MAS as well as UW NMR experiments will be presented and their use for deep insight into the structure will be demonstrated, namely for organometallic compounds and perovskites.



Dr. Libor Kobera (born 1982) received his PhD in 2014 at University of Chemistry and Technology Prague, Czech Rep., with a thesis: The preparation and structural characterization of hybrid inorganic-organic polymer systems; the development and application of solid state NMR techniques. After post-doctoral studies at University of Ottawa, Canada, he has returned to the Institute of Macromolecular Chemistry, Prague. Although he is still active in structural research of polymers materials, the core of his research activities today is focused on framework materials such as MOFs, zeolites and perovskites. Current projects involve NMR analysis of quadrupolar nuclei especially the development of NMR techniques for UW NMR spectroscopy; recording and analyzing of ultra-wide NMR lines. Libor has so far published >50 peer-reviewed journal publications. He is involved in several research grants and collaboration projects.